1-Nitropropane

108-03-2 | DTXSID1020980

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -87.7 °C

Global applicability domain: Inside

Local applicability domain index: 6.81e-01

Confidence level: 4.88e-01

Nearest Neighbors from the Training Set

Image not found
1-Nitropropane
Measured: -108
Predicted: -87.7

Image not found
2-Nitropropane
Measured: -91.3
Predicted: -84.6

Image not found
1-Nitrobutane
Measured: -81.3
Predicted: -46.4

Image not found
Propane, 2-methyl-1-nitro-
Measured: -76.9
Predicted: -40.3

Image not found
Propane, 2-methyl-2-nitro-
Measured: 26.2
Predicted: -20.5